

2-Isopropyl-6-methyl-4-pyrimidone
2814-20-2 | DTXSID1027502

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 131 °C

Global applicability domain: Inside

Local applicability domain index: 6.36e-01

Confidence level: 4.01e-01

Nearest Neighbors from the Training Set

Image not found

2-Isopropyl-6-methyl-4-pyrimidone

Measured: 173

Predicted: 131

Image not found

Cotinine

Measured: 41.0

Predicted: 96.3

Image not found

N,N-Diethylnicotinamide

Measured: 25.0

Predicted: 60.6

Image not found

O-Methylbufotenine

Measured: 69.5

Predicted: 80.6